=>
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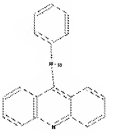
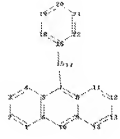




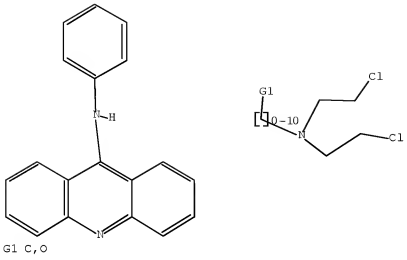
chain nodes :
15 17 23 24 25 26 27 28 29 30 31
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 16 18 19 20 21 22
chain bonds :
7-15 15-16 15-17 23-24 23-27 23-30 24-25 25-26 27-28 28-29 30-31
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 8-11 9-10 9-14 11-12 12-13
13-14 16-18 16-22 18-19 19-20 20-21 21-22
exact/norm bonds :
7-15 15-16 23-24 23-27 23-30 30-31
exact bonds :
15-17 24-25 25-26 27-28 28-29
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 8-11 9-10 9-14 11-12 12-13
13-14 16-18 16-22 18-19 19-20 20-21 21-22

G1:C,O

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS
18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS
26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

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=> s l1
SAMPLE SEARCH INITIATED 17:54:57 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -        3 TO ITERATE

100.0% PROCESSED         3 ITERATIONS                                 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            3 TO      163
PROJECTED ANSWERS:               2 TO      124

L2            2 SEA SSS SAM L1

=> s l1 ful
FULL SEARCH INITIATED 17:55:01 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -       96 TO ITERATE

100.0% PROCESSED        96 ITERATIONS                                66 ANSWERS
SEARCH TIME: 00.00.01

L3           66 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     178.36     178.57

FILE 'CAPLUS' ENTERED AT 17:55:04 ON 12 JUN 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 12 Jun 2008 VOL 148 ISS 24
FILE LAST UPDATED: 11 Jun 2008 (20080611/ED)

=> s l3
L4 6 L3

=> d abs fbib hitstr 1-6

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

AB A series of 9-(anilino)acridine and acridine derivs. bearing an alkylating N-mustard residue at C4 of the acridine chromophore were synthesized. The N-mustard pharmacophore was linked to the C4 of the acridine ring with an O-Et (O-C2), O-Pr (O-C3), or O-Bu (O-C4) spacer. It revealed that all newly synthesized compds. were very potent cytotoxic agents against human leukemia and various solid tumors in vitro. These agents did not exhibit cross-resistance against vinblastine-resistant (CCRF-CEM/VBL) or taxol-resistant (CCRF-CEM/taxol) cells. It also showed that these agents were DNA crosslinking agents rather than topoisomerase II inhibitors. Of these agents, two compds. were shown to have potent antitumor activity in nude mice bearing the human breast carcinoma MX-1 xenograft. The therapeutic efficacy of these two agents are comparable to that of taxol.

AN 2006:478646 CAPLUS Full-text

DN 145:145512

TI Potent Antitumor 9-Anilinoacridines and Acridines Bearing an Alkylating N-Mustard Residue on the Acridine Chromophore: Synthesis and Biological Activity

AU Su, Tsann-Long; Lin, Yi-Wen; Chou, Ting-Chao; Zhang, Xiuguo; Bacherikov, Valeriy A.; Chen, Ching-Huang; Liu, Leroy F.; Tsai, Tsong-Jen

CS Laboratory of Bioorganic Chemistry, Institute of Biomedical Sciences, Taipei, 115, Taiwan

SO Journal of Medicinal Chemistry (2006), 49(12), 3710-3718
CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

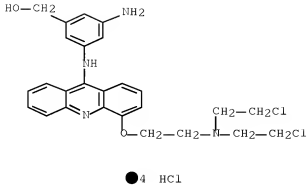
LA English

OS CASREACT 145:145512

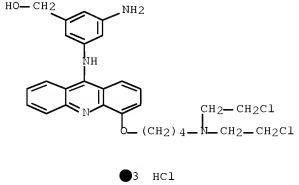
IT 898833-68-6P 898833-69-7P 898833-70-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of (amino)[[bis(chloroethyl)amino]alkoxy]acridinyl]amino]benzenemethanol derivs. and study of their antitumor activity)

RN 898833-68-6 CAPLUS

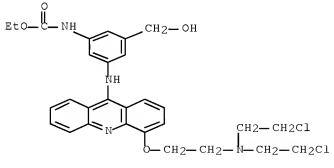
CN Benzenemethanol, 3-amino-5-[[4-[2-[bis(2-chloroethyl)amino]ethoxy]-9-acridinyl]amino]-, hydrochloride (1:4) (CA INDEX NAME)



RN 898833-69-7 CAPLUS
CN Benzenemethanol, 3-amino-5-[[4-[4-[bis(2-chloroethyl)amino]butoxy]-9-acridinyl]amino]-, hydrochloride (1:3) (CA INDEX NAME)



RN 898833-70-0 CAPLUS
CN Carbamic acid, [3-[[4-[2-[bis(2-chloroethyl)amino]ethoxy]-9-acridinyl]amino]-5-(hydroxymethyl)phenyl]-, ethyl ester (9CI) (CA INDEX NAME)

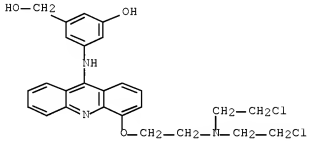


IT 898832-71-1P 898833-72-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of (hydroxy)[[bis(chloroethyl)amino]alkoxy]acridinyl]amino]benzenemethanol derivs. and study of their antitumor activity)

RN 898833-71-1 CAPLUS

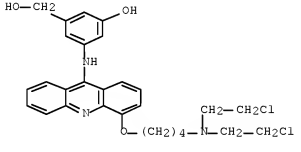
CN Benzenemethanol, 3-[[4-[2-[bis(2-chloroethyl)amino]ethoxy]-9-acridinyl]amino]-5-hydroxy-, hydrochloride (1:2) (CA INDEX NAME)



●2 HCl

RN 898833-72-2 CAPLUS

CN Benzenemethanol, 3-[[4-[4-[bis(2-chloroethyl)amino]butoxy]-9-acridinyl]amino]-5-hydroxy-, hydrochloride (2:5) (CA INDEX NAME)



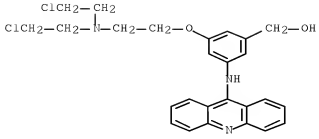
●5/2 HCl

IT 774234-08-1

RL: PAC (Pharmacological activity); BIOL (Biological study)
(preparation of (phenylamino)acridine derivs. and N-alkyl mustard group-containing acridine derivs. and study of their antitumor activity in comparison with (acridinylamino)[[bis(chloroethyl)amino]ethoxy]benzenemethanol)

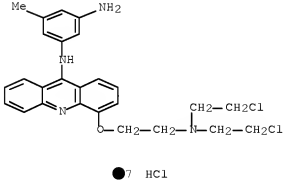
RN 774234-08-1 CAPLUS

CN Benzenemethanol, 3-(9-acridinylamino)-5-[2-[bis(2-chloroethyl)amino]ethoxy]- (CA INDEX NAME)



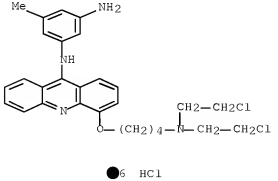
IT 898833-73-3P 898833-74-4P 898833-75-5P
898833-76-6P 898833-77-7P 898833-78-8P
898833-79-9P 898833-80-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of [[bis(chloroethyl)amino]alkoxy]acridinyl]benzenediamine derivs. and study of their antitumor activity)

RN 898833-73-3 CAPLUS
CN 1,3-Benzenediamine, N1-[4-[2-[bis(2-chloroethyl)amino]ethoxy]-9-acridinyl]-5-methyl-, hydrochloride (1:7) (CA INDEX NAME)



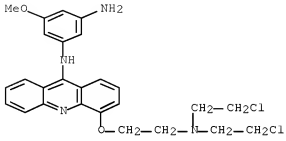
●7 HCl

RN 898833-74-4 CAPLUS
CN 1,3-Benzenediamine, N1-[4-[4-[bis(2-chloroethyl)amino]butoxy]-9-acridinyl]-5-methyl-, hydrochloride (1:6) (CA INDEX NAME)



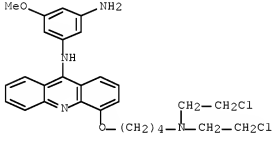
●6 HCl

RN 898833-75-5 CAPLUS
CN 1,3-Benzenediamine, N1-[4-[2-[bis(2-chloroethyl)amino]ethoxy]-9-acridinyl]-5-methoxy-, hydrochloride (1:4) (CA INDEX NAME)



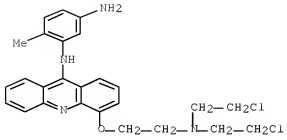
●4 HCl

RN 898833-76-6 CAPLUS
CN 1,3-Benzenediamine, N1-[4-[4-[bis(2-chloroethyl)amino]butoxy]-9-acridinyl]-5-methoxy-, hydrochloride (1:4) (CA INDEX NAME)



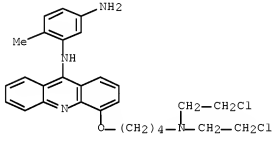
●4 HCl

RN 898833-77-7 CAPLUS
CN 1,3-Benzenediamine, N3-[4-[2-[bis(2-chloroethyl)amino]ethoxy]-9-acridinyl]-4-methyl-, hydrochloride (1:4) (CA INDEX NAME)



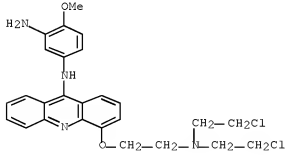
●4 HCl

RN 898833-78-8 CAPLUS
CN 1,3-Benzenediamine, N3-[4-[4-[bis(2-chloroethyl)amino]butoxy]-9-acridinyl]-4-methyl-, hydrochloride (1:4) (CA INDEX NAME)



●4 HCl

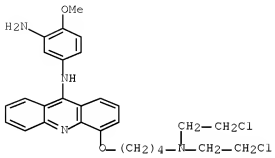
RN 898833-79-9 CAPLUS
CN 1,3-Benzenediamine, N1-[4-[2-[bis(2-chloroethyl)amino]ethoxy]-9-acridinyl]-4-methoxy-, hydrochloride (1:4) (CA INDEX NAME)



●4 HCl

RN 898833-80-2 CAPLUS
CN 1,3-Benzenediamine, N1-[4-[4-[bis(2-chloroethyl)amino]butoxy]-9-acridinyl]-

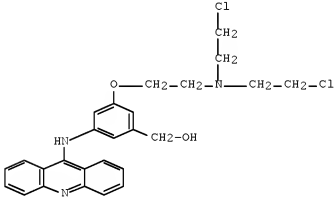
4-methoxy-, hydrochloride (10:67) (CA INDEX NAME)



●67/10 HCl

RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
GI



I

AB A series of N-mustard derivs. of 9-anilinoacridine was synthesized for antitumor and structure-activity relationship studies. The alkylating N-mustard residue was linked to the C-3' or C-4' position of the anilino ring with an O-ethylene (O-C2), O-butylene (O-C4), and methylene (C1) spacer. All of the new N-mustard derivs. exhibited significant cytotoxicity in inhibiting human lymphoblastic leukemic cells (CCRF-CEM) in culture. Of these agents, (3-(acridin-9-ylamino)-5-{2-[bis (2-chloroethyl)amino]ethoxy}phenyl)methanol (I) was subjected to antitumor studies, resulting in an approx. 100-fold more potent effect than its parent analog 3-(9-acridinylamino)-5-hydroxymethylaniline (AHMA) in inhibiting the growth of human lymphoblastic leukemic cells (CCRF-CEM) in vitro. This agent did not exhibit cross-resistance against vinblastine-resistant (CCRF-CEM/VBL) or Taxol-resistant (CCRF-CEM/Taxol) cells. Remarkably, the therapeutic effect of I at a dose as

low as one tenth of the Taxol therapeutic dose [i.e., 1-2 mg/kg (Q3D + 7) or 3 mg/kg (Q4D + 5); i.v. injection] on nude mice bearing human breast carcinoma MX-1 xenografts resulted in complete tumor remission in two out of three mice. Furthermore, I yielded xenograft tumor suppression of 81-96% using human T-cell acute lymphoblastic leukemia CCRF-CEM, colon carcinoma HCT-116, and ovarian adenocarcinoma SK-OV-3 tumor models.

AN 2005:464998 CAPLUS Full-text

DN 143:125829

TI Potent antitumor 9-anilinoacridines bearing an alkylating N-mustard residue on the anilino ring: synthesis and biological activity

AU Bacherikov, Valeriy A.; Chou, Ting-Chao; Dong, Hua-Jin; Zhang, Xiuguo; Chen, Ching-Huang; Lin, Yi-Wen; Tsai, Tsong-Jen; Lee, Rong-Zau; Liu, Leroy F.; Su, Tsann-Long

CS Laboratory of Bioorganic Chemistry, Institute of Biomedical Sciences, Academia Sinica, Taipei, 115, Taiwan

SO Bioorganic & Medicinal Chemistry (2005), 13(12), 3993-4006
CODEN: BMECEP; ISSN: 0968-0896

PB Elsevier Ltd.

DT Journal

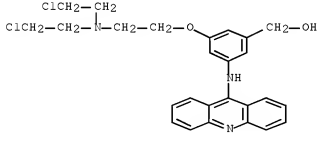
LA English

OS CASREACT 143:125829

IT 774234-08-1P 858136-02-4P 858136-03-5P
858136-04-6P 858136-05-7P 858136-06-8P
858136-07-9P 858136-08-0P 858136-09-1P
858136-10-4P 858136-11-5P 858136-12-6P
858136-13-7P 858136-14-8P 858136-15-9P
858136-16-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(antitumor 9-anilinoacridines bearing an alkylating N-mustard residue on the anilino ring)

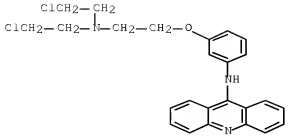
RN 774234-08-1 CAPLUS

CN Benzenemethanol, 3-(9-acridinylamino)-5-[2-[bis(2-chloroethyl)amino]ethoxy]- (CA INDEX NAME)



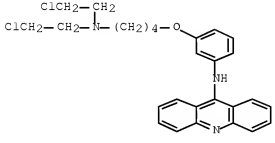
RN 858136-02-4 CAPLUS

CN 9-Acridinamine, N-[3-[2-[bis(2-chloroethyl)amino]ethoxy]phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



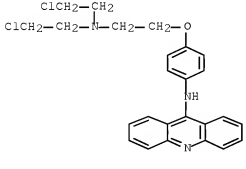
● HCl

RN 858136-03-5 CAPLUS
CN 9-Acridinamine, N-[3-[4-[bis(2-chloroethyl)amino]butoxy]phenyl]-, hydrochloride (1:2) (CA INDEX NAME)



●2 HCl

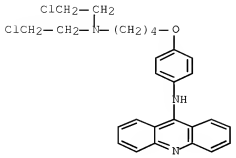
RN 858136-04-6 CAPLUS
CN 9-Acridinamine, N-[4-[2-[bis(2-chloroethyl)amino]ethoxy]phenyl]-, hydrochloride (1:2) (CA INDEX NAME)



●2 HCl

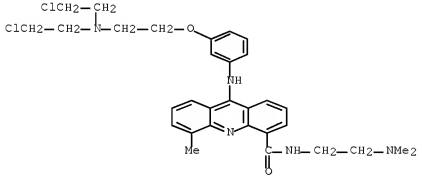
RN 858136-05-7 CAPLUS
CN 9-Acridinamine, N-[4-[4-[bis(2-chloroethyl)amino]butoxy]phenyl]-,

hydrochloride (1:3) (CA INDEX NAME)



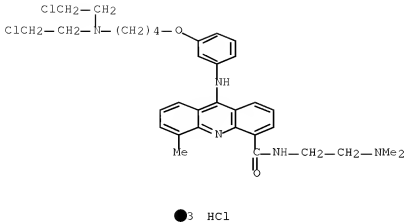
●3 HCl

RN 858136-06-8 CAPLUS
CN 4-Acridinecarboxamide, 9-[[3-[2-[bis(2-chloroethyl)amino]ethoxy]phenyl]amino]-N-[2-(dimethylamino)ethyl]-5-methyl-, hydrochloride (1:4) (CA INDEX NAME)



●4 HCl

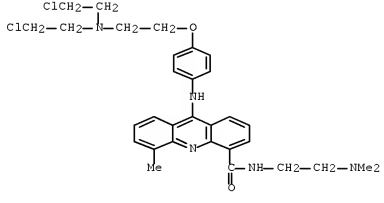
RN 858136-07-9 CAPLUS
CN 4-Acridinecarboxamide, 9-[[3-[4-[bis(2-chloroethyl)amino]butoxy]phenyl]amino]-N-[2-(dimethylamino)ethyl]-5-methyl-, hydrochloride (1:3) (CA INDEX NAME)



●3 HCl

RN 858136-08-0 CAPLUS
CN 4-Acridinecarboxamide, 9-[[4-[2-[bis(2-chloroethyl)amino]ethoxy]phenyl]amino]-N-[2-(dimethylamino)ethyl]-5-methyl-, hydrochloride (2:5) (CA INDEX NAME)

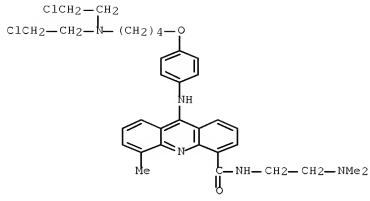
PAGE 1-A



PAGE 2-A

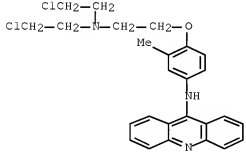
●5/2 HCl

RN 858136-09-1 CAPLUS
CN 4-Acridinecarboxamide, 9-[[4-[4-[bis(2-chloroethyl)amino]butoxy]phenyl]amino]-N-[2-(dimethylamino)ethyl]-5-methyl-, hydrochloride (2:3) (CA INDEX NAME)



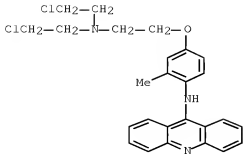
●3/2 HCl

RN 858136-10-4 CAPLUS
CN 9-Acridinamine, N-[4-[2-[bis(2-chloroethyl)amino]ethoxy]-3-methylphenyl]-, hydrochloride (2:3) (CA INDEX NAME)



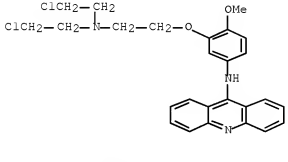
●3/2 HCl

RN 858136-11-5 CAPLUS
CN 9-Acridinamine, N-[4-[2-[bis(2-chloroethyl)amino]ethoxy]-2-methylphenyl]-, hydrochloride (2:3) (CA INDEX NAME)



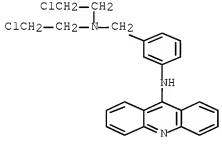
●3/2 HCl

RN 858136-12-6 CAPLUS
CN 9-Acridinamine, N-[3-[2-[bis(2-chloroethyl)amino]ethoxy]-4-methoxyphenyl]-, hydrochloride (4:5) (CA INDEX NAME)



●5/4 HCl

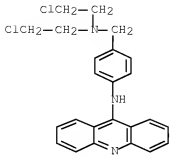
RN 858136-13-7 CAPLUS
CN 9-Acridinamine, N-[3-[[bis(2-chloroethyl)amino]methyl]phenyl]-, hydrochloride (1:2) (CA INDEX NAME)



●2 HCl

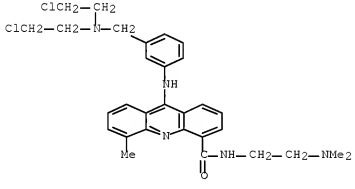
RN 858136-14-8 CAPLUS
CN 9-Acridinamine, N-[4-[[bis(2-chloroethyl)amino]methyl]phenyl]-,

hydrochloride (1:2) (CA INDEX NAME)



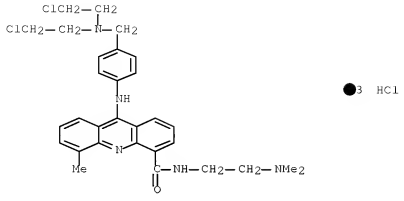
●2 HCl

RN 858136-15-9 CAPLUS
CN 4-Acridinecarboxamide, 9-[[3-[[bis(2-chloroethyl)amino]methyl]phenyl]amino]-N-[2-(dimethylamino)ethyl]-5-methyl-, hydrochloride (1:3) (CA INDEX NAME)



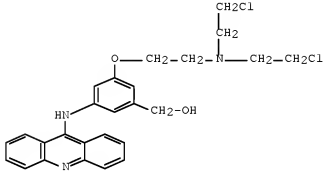
●3 HCl

RN 858136-16-0 CAPLUS
CN 4-Acridinecarboxamide, 9-[[4-[[bis(2-chloroethyl)amino]methyl]phenyl]amino]-N-[2-(dimethylamino)ethyl]-5-methyl-, hydrochloride (1:3) (CA INDEX NAME)



RE.CNT 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
GI



I

AB A series of 9-anilinoacridine N-mustard derivs., in which the alkylating N-mustard residue was linked to the C-3' or C-4' position of the anilino ring with an O-ethylene spacer, was synthesized and evaluated for cytotoxicity against human lymphoblastic leukemic cells (CCRF-CEM) in culture. The results showed that all of the new compds. exhibited potent cytotoxicity with IC50 values ranging from 0.002 to 0.7 μM, which were as potent or significantly more potent than 3-(9-acridinylamino)-5- hydroxymethylaniline (AHMA). Compound I did not exhibit cross-resistance against both vinblastine-resistant (CCRF-CEM/VBL) and taxol-resistant (CCRF-CEM/taxol) cells. Addnl., compound I demonstrated potent antitumor effect in nude mice bearing human breast carcinoma MX-1 xenografts, resulting in complete tumor remission in two out of three mice at the maximal dose of 1-2mg/kg (Q3D+7) or 3mg/kg (Q4D+5) via i.v. injection.

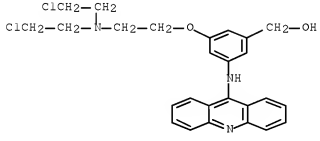
AN 2004:689256 CAPLUS Full-text

DN 141:342864

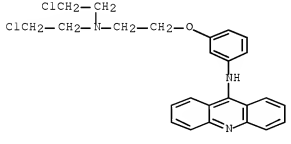
TI Potent antitumor N-mustard derivatives of 9-anilinoacridine, synthesis and antitumor evaluation

AU Bacherikov, Valeriy A.; Chou, Ting-Chao; Dong, Hua-Jin; Chen, Ching-Huang;

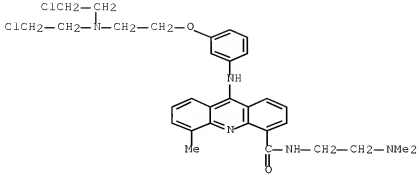
Lin, Yi-Wen; Tsai, Tsong-Jen; Su, Tsann-Long
CS Laboratory of Bioorganic Chemistry, Institute of Biomedical Sciences, Academia Sinica, Taipei, 115, Taiwan
SO Bioorganic & Medicinal Chemistry Letters (2004), 14(18), 4719-4722
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier B.V.
DT Journal
LA English
OS CASREACT 141:342864
IT 774234-08-1P 774234-11-6P 774234-12-7P
774234-13-8P 774234-14-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(antitumor N-mustard derivs. of anilinoacridine)
RN 774234-08-1 CAPLUS
CN Benzenemethanol, 3-(9-acridinylamino)-5-[2-[bis(2-chloroethyl)amino]ethoxy]- (CA INDEX NAME)



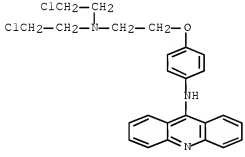
RN 774234-11-6 CAPLUS
CN 9-Acridinamine, N-[3-[2-[bis(2-chloroethyl)amino]ethoxy]phenyl]- (CA INDEX NAME)



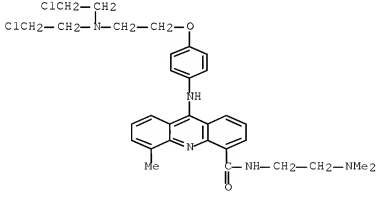
RN 774234-12-7 CAPLUS
CN 4-Acridinecarboxamide, 9-[[3-[2-[bis(2-chloroethyl)amino]ethoxy]phenyl]amino]-N-[2-(dimethylamino)ethyl]-5-methyl- (CA INDEX NAME)



RN 774234-13-8 CAPLUS
CN 9-Acridinamine, N-[4-[2-[bis(2-chloroethyl)amino]ethoxy]phenyl]- (CA INDEX NAME)



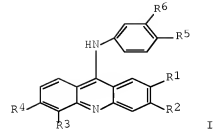
RN 774234-14-9 CAPLUS
CN 4-Acridinecarboxamide, 9-[[4-[2-[bis(2-chloroethyl)amino]ethoxy]phenyl]amino]-N-[2-(dimethylamino)ethyl]-5-methyl- (CA INDEX NAME)



RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

GI



I

AB A possible mode of action involving electron transfer is advanced for the 9-anilinoacridines [I; R1 = H, OMe; R2 and R4 = H, Cl; R3 = H, Me; R5 = H, OH, OEt, CO2H; R6 = OH, CH2NEt2, CH2N(CH2)4, CH2N(CH2CH2Cl)2, CH2N[(CH2)7Me]2]. The mechanism entails formation of toxic oxy radicals which destroy the neoplasm. Cyclic voltammetry was performed on iminium type ions derived by protonation of the acridines. Redns. were generally reversible with potentials of about -0.60 V. Involvement of quinoidal metabolites is also a possibility. The relationship of electrochem. behavior to structure and physiol. activity is addressed.

AN 1987:628450 CAPLUS Full-text
DN 107:228450
OREF 107:36495a,36498a

TI Electron transfer-oxy radical mechanism for anticancer agents: 9-anilinoacridines

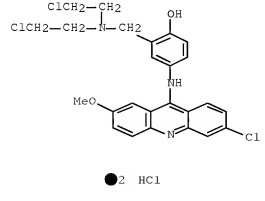
AU Kovacic, P.; Ames, J. R.; Ryan, M. D.
CS Dep. Chem., Univ. Wisconsin, Milwaukee, WI, 53201, USA

SO Anti-Cancer Drug Design (1987), 2(1), 37-46
CODEN: ACDDEA; ISSN: 0266-9536
DT Journal
LA English

IT 111393-51-2
RL: BIOL (Biological study)
(electron transfer-oxy radical mechanisms for antitumor, structure in relation to)

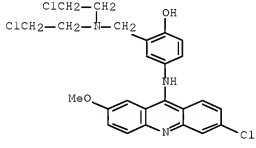
RN 111393-51-2 CAPLUS

CN Phenol, 2-[[bis(2-chloroethyl)amino]methyl]-4-[(6-chloro-2-methoxy-9-acridinyl)amino]-, dihydrochloride (9CI) (CA INDEX NAME)

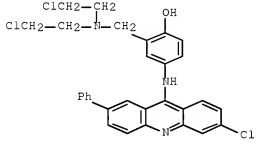


●2 HCl

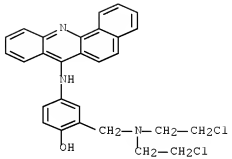
L4 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
AB cf. CA 54, 6954d. This indexed compilation contains information concerning 1816 compds. tested.
AN 1960:131417 CAPLUS Full-text
DN 54:131417
OREF 54:25245g
TI Cancer chemotherapy screening data. VII
AU Leiter, Joseph
SO Cancer Research (1960), 20(No. 7,Pt. 2), 471-684
CODEN: CNREA8; ISSN: 0008-5472
DT Journal
LA Unavailable
IT 102892-27-3, o-Cresol, α-[bis(2-chloroethyl)amino]-4-[(6-chloro-2-methoxy-9-acridinyl)amino]- 115918-36-0, o-Cresol, α-[bis(2-chloroethyl)amino]-4-[(6-chloro-2-phenyl-9-acridinyl)amino]- 121814-84-4, o-Cresol, 4-benz[c]acridin-7-ylamino-α-[bis(2-chloroethyl)amino]-
(as cancer inhibitor)
RN 102892-27-3 CAPLUS
CN Phenol, 2-[[bis(2-chloroethyl)amino]methyl]-4-[(6-chloro-2-methoxy-9-acridinyl)amino]- (CA INDEX NAME)



RN 115918-36-0 CAPLUS
CN o-Cresol, α-[bis(2-chloroethyl)amino]-4-[(6-chloro-2-phenyl-9-acridinyl)amino]- (6CI) (CA INDEX NAME)



RN 121814-84-4 CAPLUS
CN o-Cresol, 4-benz[c]acridin-7-ylamino-α-[bis(2-chloroethyl)amino]- (6CI) (CA INDEX NAME)



L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

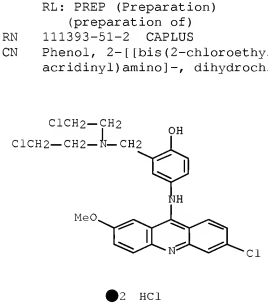
AB Diaminocresols and salts thereof, useful as agricultural fungicides against Alternaria solani, are prepared by converting the alcoholic hydroxyl groups in a substituted cresol to the chloride with SOCl2. 2,2'-[5-(7-Chloro-4-quinolylamino)-2-hydroxybenzylimino]diethanol (I) is prepared as follows: 30 g. paraformaldehyde, 105 g. diethanolamine, and 100 ml. EtOH is boiled to a clear solution to which is added a hot solution of 151 g. 4'-hydroxyacetanilide in 100 ml. EtOH. The mixture is refluxed 3 hrs., 500 ml. 1:1-HCl added, refluxed 2 hrs., the residue dried thoroughly and treated with 198 g. 4,7-dichloroquinoline and 400 g. PhOH and heated 3 hrs. at 130-140°. The melt is acidified with alc. HCl, precipitated with five vols. of acetone to a gum which is triturated with Et2O to a granular solid. Acetone containing a slight excess of NH4OH extracts the base. The acetone solution is decolorized with C, concentrated to 2 l. and diluted with 1.5 vols. hot H2O to give yellow I, m. 193-4° (50% EtOH). 4,7-Dichloroquinoline (81.5 g.), 68.8 g. p-methylaminophenol sulfate, and 150 g. PhOH is heated 2 hrs. at 140°, then heated in succession with a few drops of alc. HCl, one volume acetone and 5 vols. Et2O. The precipitated red oil is triturated with anhydrous Et2O and with excess saturated NaHCO3 solution The precipitate collected by filtration, washed with ether, saturated NaHCO3 and water, is dried and digested with 400 ml. 95% EtOH to give 4-[(7-chloro-4-quinolyl)methylamino]phenol (II), m. 256-8° (EtOH). A mixture of 15.7 g. diethanolamine, 4.5 g. paraformaldehyde, and 100 ml. PrOH is heated to a solution which is added to a suspension of 27.5 g. II in 250 ml. PrOH and refluxed 4 hrs. The mixture is repeatedly filtered hot after boiling with fresh amts. of diethanolamine-paraformaldehyde solution The combined filtrate is concentrated in vacuo to a sirup which is made alkaline with NaOH and extracted with CHCl3. The CHCl3 extract, washed with 5% NaOH solution, water, is evaporated in vacuo to a gum. The alc. solution of the residue is treated with C and excess alc. HCl and poured into 2 l. Et2O to give hygroscopic, yellow 2,2'-{5-[(7-chloro-4-quinolyl)amino]-2- hydroxybenzylimino}diethanol-2HCl.3/4H2O (III) of indefinite m.p. Hydrated 2,2'-[5-(benz[c]acridin-7-ylamino)-2-hydroxybenzylimino]diethanol- 2HCl (IV), m. 105-10° (decomposition), is prepared likewise from 29.9 g. 2,2'-(5-amino-2-hydroxybenzylimino)diethanol-2HCl, 29.9 g. 7-chlorobenz[c]acridine and 75 g. phenol. I (5.8 g.) is added in portions to 20 ml. SOCl2 with stirring. After 16 hrs. at room temperature excess SOCl2 is removed by decantation, the brown oily residue is taken up in absolute EtOH, treated with C, filtered and evaporated to about 50 ml. The cooled alc. solution is poured with vigorous stirring into 500 ml. anhydrous Et2O to give α-[bis(2-chloroethyl)amino]-4-(7-chloro-4-quinolylamino)-o- cresol-2HCl.1.5H2O, m. 120° (decomposition). In other examples the volume SOCl2, weight of starting heterocyclic alc., and the product and m.p. obtained are: 30 ml., 4 g. 2,2'-[5-(benzo[h]quinolin-4-

ylamino)-2- hydroxybenzylimino]diethanol, 4-(benzo[h]quinolin-4-ylamino)-α-[bis(2-chloroethyl)amino]-o-cresol-2HCl, -; 65 ml., 8.0 g. 2,2'-[5-(benzo[f]quinolin-1-ylamino)-2-hydroxybenzylimino]diethanol, 4-(benzo[f]quinolin-1-ylamino)-α-[bis(2-chloroethyl)amino]-o- cresol-2HCl, -; 20 ml., 4.7 g. III, α-[bis(2-chloroethyl)amino]-4- [(7-chloro-4-quinolyl)methylamino]-o-cresol-2HCl, -; 200 ml., 36.8 g. 2,2'-[5-(6-chloro-2-methoxyacridin-9-ylamino)-2- hydroxybenzylimino]diethanol, α-[bis(2-chloroethyl)amino]-4-(6- chloro-2-methoxy-9-acridinylamino)-o-cresol-2HCl, 195-6° (decomposition); 100 ml., 5.3 g. 2,2'-[5-(benz[b]acridin-12-ylamino)-2-hydroxybenzylimino]diethanol-2HCl, 4-(benz[b]acridin-12-ylamino)-α- [bis(2-chloroethyl)amino]-o-cresol-2HCl, -; 150 ml., 10.6 g. IV, 4-(benz[c]-acridin-7-ylamino)-α-[bis(2-chloroethyl)amino]-o- cresol-2HCl, -; 400 ml., 21.2 g. 2,2'-[5-(benz[a]acridin-12-ylamino)-2- hydroxybenzylimino]diethanol-2HCl, 4-(benz[a]acridin-12-ylamino)-α- [bis(2-chloroethyl)amino]-o-cresol-2HCl, -.

AN 1959:89542 CAPLUS Full-text
DN 53:89542
OREF 53:16165f-i,16166a-e
TI Benzoquinolylamino-2-[bis(β-chloroethyl)aminomethyl]phenols
IN Elslager, E. F.; Tendick, F. H.
PA Parke, Davis & Co.
DT Patent
LA Unavailable
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2883382		19590421	US 1957-680928	19570829

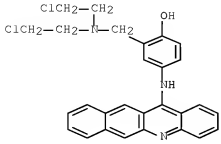
IT 111393-51-2P, o-Cresol, α-[bis(2-chloroethyl)amino]-4-[(6-chloro-2-methoxy-9-acridinyl)amino]-, dihydrochloride 121814-85-5P, o-Cresol, 4-benz[b]acridin-12-ylamino-α-[bis(2-chloroethyl)amino]-, dihydrochloride 122021-13-0P, o-Cresol, 4-benz[c]acridin-7-ylamino-α-[bis(2-chloroethyl)amino]-, dihydrochloride 859924-40-6P, o-Cresol, 4-benz[a]acridin-12-ylamino-α-[bis(2-chloroethyl)amino]-
RL: PREP (Preparation)
(preparation of)
RN 111393-51-2 CAPLUS
CN Phenol, 2-[[bis(2-chloroethyl)amino]methyl]-4-[(6-chloro-2-methoxy-9-acridinyl)amino]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

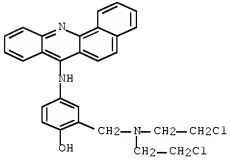
RN 121814-85-5 CAPLUS
CN o-Cresol, 4-benz[b]acridin-12-ylamino-α-[bis(2-chloroethyl)amino]-,

dihydrochloride (6CI) (CA INDEX NAME)



●2 HCl

RN 122021-13-0 CAPLUS
CN o-Cresol, 4-benz[c]acridin-7-ylamino-α-[bis(2-chloroethyl)amino]-,
dihydrochloride (6CI) (CA INDEX NAME)



●2 HCl

RN 859924-40-6 CAPLUS
CN Phenol, 4-(benz[a]acridin-12-ylamino)-2-[[bis(2-chloroethyl)amino]methyl]-
(CA INDEX NAME)